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This work presents a methodology for calculating reaction rates in a reactive transport system under kinetic and equilibrium conditions for a bidimensional fully saturated homogeneous aquifer [GRDMOMAS,2006]. The system considered is the scenario of precipitation/dissolution of two minerals [Donado et al, In preparation] $B_4^{(s)}$ and $B_5^{(s)}$ in the presence of three aqueous species, B_1, B_2 and B_3, governed by the reactions

$B_1+B_2 \rightleftharpoons B_4^{(s)}$ [1]

$B_1+B_3 \rightleftharpoons B_5^{(s)}$ [2]

Reaction ([1]) is considered to occur in instantaneous equilibrium, while reaction ([2]) is considered to be a slow (i.e., kinetic) reaction [Cirpka and Valocchi, 2007]. Using the approach proposed by Molins et al. [Water Resour. Res., 40(10), W10301, doi:10.1029/2003WR002970, 2004], two linear combinations of the concentrations of the reacting species, known as the conservative and kinetic components u and u_k, are defined in order to decouple the equilibrium reaction from the kinetic one. This way the set of equations which describes the reactive transport system is reduced to two partial differential equations; the first one of them is a second-order linear homogeneous parabolic partial differential equation solely in terms of the conservative component u, which can be solved separately, while the second one is a second-order non-linear non-homogeneous parabolic partial differential equation in terms of both the conservative and kinetic components.

An approximate numerical solution of the aforementioned partial differential equations is obtained by applying a mixed solution by means of the finite elements method for flow and finite differences method for transport. A bilinear grid is used for discretizing the flow-reaction domain while the Crank-Nicholson implicit scheme is used for the temporal integration of the equations. The nonlinearity of the second partial differential equation is treated using a predictor-corrector algorithm.

The behaviour of the reactive transport system is evaluated in term of two of its chemical and hydrodynamic parameters: The relationship among diffusive and reactive times (Damkhöler number) and the quotient of the transverse and longitudinal diffusivity/dispersivity of the aquifer. It is observed that the spatial-temporal variation of the concentration of B_1 is independent of Damkhöler number, while the behaviour of the concentration of B_3 approaches equilibrium with B_1 as Damkhöler number rises. Also, results show that the aquifer requires a certain diffusivity/dispersivity so that two reaction fronts are juxtaposed.

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